

**SIMULATION STUDIES FOR SURFACES
AND MATERIALS STRENGTH**

AMES
GRANT

1N-72-CR

172901

P-25

Semiannual Progress Report
for
Cooperative Agreement NCC2-297

for the period
May 1, 1988 - October 31, 1988

Submitted to

National Aeronautics and Space Administration
Ames Research Center
Moffett Field, California 94035

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(NASA-CR-183378) SIMULATION STUDIES FOR
SURFACES AND MATERIALS STRENGTH Semiannual
Progress Report, 1 May - 31 Oct. 1988
(Eloret Corp.) 25 p

CSSL 20H

N89-14824

Unclas
G3/72 0172901

During this six month period of the program investigations were carried out in two general areas. (i) Energy barriers and structural transitions between isomers of small Al clusters were investigated. In this study an empirical potential function which was parametrized based on accurate first principle results was employed. (ii) A comparative study was conducted to investigate the applicability of most commonly employed model potential functions in calculating various bulk, surface and small cluster properties.

I. Calculation of Energy Barriers and Transition Structures for Small Al Clusters.

A model potential energy function fitted to high level *ab initio* results is used for the first time to calculate saddle point configurations and energies between low lying structures of Al₄, Al₅ and Al₆. For these clusters, energy barriers for structural isomerizations were found to be of varying heights. In general, barriers between high-symmetry equilibrium structures are low indicating that for those cases isomerization reactions in the gas-phase may take place at lower temperatures. On the other hand, calculations indicate that barriers between two- and three-dimensional forms are high which may affect the equilibration process in the gas-phase.

This work has been presented in the *Fourth International Symposium on Small Particles and Inorganic Clusters* held in Aix-en-Provence, France, on July 5 - 9, 1988. Appendix I includes the manuscript which will be published in "Atoms, Molecules and Clusters" (Zeitschrift fur Physik D).

II. Comparison of Interatomic Potentials Based on Multi-Body Interactions

In this study, four most commonly used model potentials comprising two- and three-body interactions were analyzed comparatively. We included " Tersoff", " Tersoff-Dodson", " Stillenger-Weber" and " Lennard-Jones-Axilrod-Teller" potentials, and investigated their capabilities in reproducing various bulk, surface and small cluster properties of some selected elements. Applicability and limitations of each potential function were delineated and discussed separately. In general, structural properties calculated by these functions were found to be in better agreement with experiment than corresponding energy-related properties.

The first part of this study dealing with properties of silicon has been now completed and the manuscript has been sent for publication. A shortend version of this manuscript is presented in Appendix II.

APPENDIX I.

Energy Barriers and Structural Transitions of Small Al Clusters

Recent experimental and theoretical investigations on small clusters indicate that certain microclusters exhibit isomeric transformations in the gas phase [1-7]. In order to thoroughly understand and analyze those isomerization processes, all the stationary points (at least for the low-lying configurations) of the potential energy surface associated with the cluster, must be estimated [8]. Stationary points include not only the minima of the surface, but also saddle point configurations [9]. At the present time, highly accurate calculations based on *ab initio* methods, are possible only for geometry optimizations of relatively smaller clusters [10]. A high level calculation for the lowest saddle point of paths connecting two minima, however, is a formidable job even with today's supercomputers. In this work, using a model potential energy function, which takes into account two- and three-body interactions, we calculated saddle point structures and corresponding energies between several low-lying equilibrium configurations of Al_4 , Al_5 and Al_6 . The model potential was parametrized by fitting it to highly accurate *ab initio* results and it has been shown that it is able to reproduce many equilibrium structures of small Al clusters (up to 6 atoms) with an acceptable accuracy [10]. The functional form of the potential and values of parameters are given in reference 10. Configurations corresponding to energy minima were calculated in this work, by an energy gradient method [9]. Low-lying configurations were selected from a large number of results calculated with different initial geometries. Saddle points like minima were also treated as stationary points on the energy surface. Several different paths between two configurational minima were taken into consideration and the saddle point structure corresponding to the path with the lowest barrier is reported in this study. Calculated results are summarized in Table 1.

For the Al_4 case, the two lowest minimum energy structures corresponding to three-dimensional (3d) and two-dimensional (2d) configurations, are the regular tetrahedron $(T)_4$ and the rhombus $(R)_4$ structures, respectively. The saddle point structure for the $(T)_4 \rightarrow (R)_4$ transformation is a highly distorted tetrahedron with one elongated side. The barrier for this 3d \rightarrow 2d transition was estimated as 0.0299 eV/atom.

Energetically low-lying 3d configurations for the Al_5 case are the triangular bipyramid $(TBP)_5$ which is the most compact structure and the square pyramid $(SP)_5$. The energetically most favorable Al_5 structure is the 2d close-packed $(CP)_5$ configuration. Two saddle point structures were calculated, in this case. For the transition between two 3d structures, the saddle point configuration was found to be a distorted triangular bipyramid. Its two apex atoms are shifted toward to one side of the triangular base. Calculated energy for this saddle point configuration

corresponds to a 0.0055 eV/atom barrier height for the $(TBP)_5 \rightarrow (SP)_5$ transformation. For the 3d \rightarrow 2d transition, among many possible alternatives, the path with the lowest saddle point energy was found for the $(SP)_5 \rightarrow (CP)_5$ transformation. This saddle point structure resembles very much the $(CP)_5$ but it is not planar. The barrier for this $(SP)_5 \rightarrow (CP)_5$ transition was calculated to be 0.0259 eV/atom.

For Al_6 , we considered three low-lying 3d configurations. The square bipyramid $(SBP)_6$ structure is the most compact configuration. The tripyramid $(TP)_6$ is formed by three slightly distorted tetrahedra. Structurally it is similar to $(TBP)_5$ with an additional Al atom positioned above one of its faces. The pentagonal pyramid $(PP)_6$ is the energetically most stable 3d configuration. The low-lying 2d configurations for Al_6 include the close-packed $(CP)_6$ and the triangular close-packed $(TCP)_6$ structures. Three transition structures were investigated in this case. The saddle point configuration for the $(SBP)_6 \rightarrow (TP)_6$ transition, resembles the $(TP)_6$ structure with three distorted tetrahedra. The commonly shared edge of three tetrahedra, in this configuration, was found to be considerably elongated, however, the C_{2v} symmetry was still maintained. The energy of this transition structure yields a barrier of 0.0117 eV/atom for the $(SBP)_6 \rightarrow (TP)_6$ conversion reaction. The other 3d \rightarrow 3d transformation is the $(TP)_6 \rightarrow (PP)_6$ transition. The three tetrahedra (which were the building blocks of $(TP)_6$) in this saddle point structure, were highly distorted. This is the only second order saddle point [9] found in this study. Among many paths connecting equilibrium $(TP)_6$ and $(PP)_6$ configurations no first order saddle point was found with a lower energy. The calculated energy value for this saddle point configuration produces a barrier of 0.0078 eV/atom for the $(TP)_6 \rightarrow (PP)_6$ transformation. The other saddle point structure, considered in this work, belongs to the $(PP)_6 \rightarrow (CP)_6$ transition which is a 3d \rightarrow 2d transformation. This saddle point structure is a highly distorted pentagonal pyramid. The calculated barrier height for the $(PP)_6 \rightarrow (CP)_6$ transition was found to be 0.0356 eV/atom.

For $(TBP)_5 \rightarrow (SP)_5$ and $(SBP)_6 \rightarrow (TP)_6$ transformations, barrier heights (in both forward and reverse directions) were found to be quite low. This implies that isomerization reactions can easily take place at even low temperatures, and isomers may coexist in the gas phase for a certain length of time. Energy barriers for 3d \rightarrow 2d transformations, for the cases of Al_5 and Al_6 , were found to be generally higher than 3d \rightarrow 3d transitions, even though 2d structures are energetically more stable than 3d structures. This indicates that 3d \rightarrow 2d transformation reactions for Al_5 and Al_6 would proceed much slower.

In gas-phase experiments, in general, the time necessary for a complete equilibration (including all the fragmentation and structural transformation processes) is not a simple quantity to obtain. In a cluster generation process there are many factors (such as the temperature, the type of the carrier gas, dimensions of the ex-

pansion chamber, etc.) affecting the initial formation and structural characteristics of metal atom clusters. Unfortunately, present condensation theories are generally inadequate to provide a definitive prediction about the clustering conditions of metal vapors in free jet experiments [11]. Based on purely statistical considerations, however, in the very early stages of the clustering process, the probability of a 3d cluster formation is higher than that of the formation of a 2d cluster. After the equilibration period, at relatively lower temperatures, the probability of finding a cluster in its lowest energy configuration is, of course, the highest. For the Al_5 case, for example, let us compare $(SP)_5 \rightarrow (CP)_5$ and $(SP)_5 \rightarrow (TBP)_5$ transformations which are 3d \rightarrow 2d and 3d \rightarrow 3d processes, respectively. If preexponential factors of these processes are assumed to be approximately equal, then, based on the absolute rate theory (say, at $T \approx 300^\circ\text{K}$) the rate for the $(SP)_5 \rightarrow (CP)_5$ reaction is more than 100 times slower than the rate of the $(SP)_5 \rightarrow (TBP)_5$ transformation. (For transition energies see Table 1). This indicates that even though the low energy structure of Al_5 is planar, the newly formed Al_5 may remain 3d, fluctuating back and forth between $(SP)_5$ and $(TBP)_5$ configurations a great many times before the complete equilibration. It has already been shown that kinetics may play a major role in many of the processes occurring in the gas-phase [12]. In particular, if the lowest energy structure of a cluster is separated by relatively high barriers from other low-lying configurations (like Al_5 and Al_6 cases examined in this paper), then, the equilibration time may be long and it may become an important consideration in cluster beam experiments. Barrier heights between isomers may also play an important role in the kinetics of fragmentation which is an important process affecting the gas-phase composition. Among many isomeric configurations of a cluster perhaps one (or, a few) isomeric structure(s) may undergo to a fragmentation process. Accordingly, the fragmentation depends on the concentration of a particular isomer in the beam. The rate of formation of that particular isomer (which serves as a window for the fragmentation) then, becomes an important step, and the energy barriers separating this isomer from other low-lying configurations, may control the rate of the fragmentation process in the beam.

The model potential energy function employed in this study can satisfactorily reproduce highly accurate *ab initio* results for a variety of minimum energy configurations of small Al clusters [10]. However, care should be exercised in a more quantitative interpretation of the saddle point results obtained here. This is because, at the present time, no accurate calculations based on first principles are available for the barrier heights corresponding to isomeric transformation of small Al clusters for comparison.

References

- [1] M. R. Zakin, R. O. Brickman, D. M. Cox and A. Kaldor, J. Chem. Phys., **88**, 3555 (1988).

- [2] Y. Hamrick, S. Taylor, G. W. Lemire, Z.-W. Fu, J.-C. Shui and M. D. Morse, J. Chem. Phys., **88**, 4095 (1988).
- [3] J. D. Honeycutt and H. C. Andersen, J. Phys. Chem., **91**, 4950 (1987).
- [4] R. S. Berry, T. L. Beck, H. L. Davis and J. Jellinek, "Physics and Chemistry of Small Clusters", Eds: P. Jena, B. K. Rao and S. N. Khanna (NATO ASI Series, Plenum, New York, 1987) pp. 185.
- [5] H. L. Davis, J. Jellinek and R. S. Berry, J. Chem. Phys., **86**, 6456 (1987).
- [6] T. Kondow, J. Phys. Chem., **91**, 1307 (1986).
- [7] J. Gspann, Z. Phys. D, **3**, 143 (1986).
- [8] T. Halicioglu, Surf. Scie., **197**, L233 (1988).
- [9] H. B. Schlegel, Adv. in Chem. Phys., **67**, 249 (1987).
- [10] L. G. M. Pettersson, C. W. Baucshlicher, Jr. and T. Halicioglu, J. Chem. Phys., **87**, 2205 (1987).
- [11] O. F. Hagena, Z. Phys. D, **4**, 291 (1987).
- [12] J. C. Phillips, J. Chem. Phys., **83**, 3330 (1985).

Table 1

Calculated Energies and Symmetry Groups for Equilibrated
and Transition Structures of Al Clusters

Cluster	Configuration	Energy (eV/atom)	Symmetry
Al ₄	Tetrahedral (<i>T</i>) ₄	-1.1069	<i>T_d</i>
Al ₄	[(<i>T</i>) ₄ → (<i>R</i>) ₄] [‡]	-1.0770	<i>C_{2v}</i>
Al ₄	Rhombus (<i>R</i>) ₄	-1.1255	<i>D_{2h}</i>
Al ₅	Triangular bipyramid (<i>TBP</i>) ₅	-1.2469	<i>D_{3h}</i>
Al ₅	[(<i>TBP</i>) ₅ → (<i>SP</i>) ₅] [‡]	-1.2414	<i>C_{2v}</i>
Al ₅	Square Pyramid (<i>SP</i>) ₅	-1.2431	<i>C_{4v}</i>
Al ₅	[(<i>SP</i>) ₅ → (<i>CP</i>) ₅] [‡]	-1.2172	<i>C₁</i>
Al ₅	Close-Packed (<i>CP</i>) ₅	-1.2744	<i>C_{2v}</i>
Al ₆	Square Bipyramid (<i>SBP</i>) ₆	-1.3424	<i>O_h</i>
Al ₆	[(<i>SBP</i>) ₆ → (<i>TP</i>) ₆] [‡]	-1.3307	<i>C_{2v}</i>
Al ₆	Tripyramid (<i>TP</i>) ₆	-1.3480	<i>C_{2v}</i>
Al ₆	[(<i>TP</i>) ₆ → (<i>PP</i>) ₆] [‡]	-1.3402	<i>C_s</i>
Al ₆	Pentagonal Pyramid (<i>PP</i>) ₆	-1.3709	<i>C_{5v}</i>
Al ₆	[(<i>PP</i>) ₆ → (<i>CP</i>) ₆] [‡]	-1.3353	<i>C_s</i>
Al ₆	Close-Packed (<i>CP</i>) ₆	-1.3801	<i>C_{2v}</i>
Al ₆	Triangular Close-Packed (<i>TCP</i>) ₆	-1.3926	<i>D_{3h}</i>

APPENDIX II.

Interatomic Potential Functions with Multi-body Interactions

During the last 5-6 years, perhaps due to the availability of supercomputers, simulation studies have been gaining importance at an ever increasing pace. In many areas today, computer simulations are becoming an integral part of many investigative procedures and provide help in understanding various problems at atomistic levels. This information, in turn, has been used successfully in the interpretation of many experimental results. Many of these simulation techniques, which are called atomistic level simulations, are based on empirical model potentials describing interactions among the atoms in the system [1].

The concept of model potentials, generally speaking, is based on the Born-Oppenheimer approximation [2]. If it is assumed that in the absence of external forces a function $\Phi(\vec{r}_1, \dots, \vec{r}_N)$ exists to describe the total potential energy of a system of N atoms as a function of their positions, then, without any loss of generality the function Φ can be expanded as:

$$\Phi = \phi_2 + \phi_3 + \dots + \phi_n + \dots$$

where, ϕ_2 , ϕ_3 and ϕ_n denote sums of the two-body, three-body and n -body interactions, respectively. In this so called many body expansion of Φ , it is usually believed that the series has a quick convergence, therefore, the higher moments may be neglected [2,3]. Otherwise this equation can not be employed for systems containing more than only a few atoms.

In the earlier calculations, in general, the higher terms including even the three-body part were omitted, and the total potential energy, Φ , was approximated only by the sum of two-body interactions. This approach, which may be regarded as a first order approximation, not only simplified the statistical mechanical formalisms used in calculating various thermodynamical properties, but, more importantly, it enabled many earlier researchers to run simulation calculations with relatively smaller and less powerful computers. In most of the simulation calculations which are carried out considering this first order approximation, Lennard-Jones type functions were employed to mimic two-body interactions [4,5]. Despite the fact that those so called Lennard-Jones systems may only represent rare gases where the role of many-body forces is minimal, they provided a very useful understanding about many properties and processes in a systematic way that could not be acquired easily by other means [1]. Recent studies, however, have indicated that, particularly in the case of systems containing atoms other than those with close-shell structures, this first order approximation is inappropriate and produces results inconsistent with many experiments due to neglect of many-body interactions [6,7]. In more recent simulation studies, therefore, in addition to two-body interactions, three-body interactions also are being considered in the calculation of potential energies [7,8]. It has

been well recognized that the importance of three-body interactions increases with increasing covalent character of the bonding among atoms in the system. While for rare gases the three-body part is negligibly small, for metals and in particular for semiconductors their contribution turns out to be extremely significant.

In the present work we have considered four different potential energy functions which can be expressed as separate sums of two- and three-body interactions. A comparative analysis was conducted for the Tersoff (T), Tersoff-Dodson (TD), Stillinger-Weber (SW) and Pearson-Takai-Halicioglu-Tiller (PTHT) potentials to determine their ability to reproduce various bulk, surface and small cluster properties of silicon.

Potential Functions

1. The Tersoff potential is designed specifically for calculating energetics and structure related properties of covalently bonded systems [9]. It can easily be written in sums of two- and three-body interactions. The two-body part is given by:

$$\phi_2 = \frac{1}{2} \sum_i^N \sum_{\substack{j \\ i \neq j}}^N f_c(r_{ij})(Ae^{-\lambda_1 r_{ij}} - B_o e^{-\lambda_2 r_{ij}})$$

and the three-body part is expressed as:

$$\phi_3 = \frac{1}{2} \sum_i^N \sum_{\substack{j \\ i \neq j}}^N B_o e^{-\lambda_2 r_{ij}} \left\{ 1 - \exp\left(-\frac{1}{b} \left[\sum_{\substack{k \\ k \neq i, j}}^N Q_{ijk} \right]^\eta \right) \right\}$$

with

$$Q_{ijk} = \left[\frac{f_c(r_{ik})}{f_c(r_{ij})} \right]^n \frac{\exp(n\lambda_2(r_{ij} - r_{ik}))}{c + \exp(-d \cdot \cos\Theta_{jik})}$$

This potential uses a cut-off function given by

$$f_c(r_{ij}) = 1, \quad \text{for } r_{ij} < R - D$$

$$f_c(r_{ij}) = \frac{1}{2} - \frac{1}{2} \sin\left(\frac{\pi(r_{ij} - R)}{2D}\right), \quad \text{for } R - D < r_{ij} < R + D$$

$$f_c(r_{ij}) = 0, \quad \text{for } r_{ij} > R + D$$

Parameters of this potential evaluated for Si systems are tabulated in Table 1. In his original work Tersoff [9] considered $\eta = 1$ and $\lambda_1 = 2\lambda_2$ which reduces the number

of parameters to be determined from 11 down to 9. Two of these, R and D , are used to describe the cut-off function $f_c(r)$. The parameter evaluation process was accomplished by fitting the potential function to reproduce the following six data: the cohesive energy, lattice constant and bulk modulus of bulk Si, and the cohesive energies of the Si dimer and the hypothetical simple cubic and face-centered-cubic structures as calculated by *ab initio* methods [10,11].

2. In his recent paper Dodson [12] analyzed the Tersoff potential and has concluded that the potential does a good job in reproducing many properties of silicon. However, he has discovered one important shortcoming. According to Dodson [12], the energetically most favorable structure for Si, calculated by the (T) potential was not a diamond cubic, but rather was a bcc structure with an energy value approximately 1 eV/atom lower. In order to overcome this shortcoming, Dodson has modified the (T) potential. The new form of the potential that we will refer to as the Tersoff-Dodson (TD) potential, has basically the same analytical form as the (T) potential with an exception of the parameter η which was taken to be equal to unity by Tersoff. Furthermore, λ_1 and λ_2 have been treated as independent parameters. Accordingly, the (TD) potential contains basically 11 parameters to be decided. Values of the parameters for the (TD) potential calculated by Dodson are also given in Table 1 along with the parameters of the (T) potential.

3. Stillinger and Weber [13] developed a model potential comprising two- and three-body contributions to describe interactions in solid and liquid forms of covalently bonded systems. The two-body part in this potential is expressed by:

$$\phi_2 = \sum_i^N \sum_{\substack{j \\ i < j}}^N \epsilon f_2(r_{ij}^*)$$

with,

$$f_2(r_{ij}^*) = A(B(r_{ij}^*)^{-p} - (r_{ij}^*)^{-q}) \cdot \exp(\frac{1}{r_{ij}^* - a}), \quad \text{for } r_{ij}^* < a$$

$$f_2(r_{ij}^*) = 0, \quad \text{for } r_{ij}^* > a$$

where, $r_{ij}^* = r_{ij}/\sigma$, and r_{ij} is the distance between the i 'th and j 'th atoms.

The three-body part is given by:

$$\phi_3 = \sum_i^N \sum_{\substack{j \\ i < j < k}}^N \sum_k^N \epsilon f_3(r_{ij}^*, r_{ik}^*, r_{jk}^*)$$

with,

$$f_3(r_{ij}^*, r_{ik}^*, r_{jk}^*) = h(r_{ij}^*, r_{ik}^*, \theta_{jik}) + h(r_{ji}^*, r_{jk}^*, \theta_{ijk}) + h(r_{ki}^*, r_{kj}^*, \theta_{ikj})$$

where, θ_{jik} represents the angle at the vertex i between the sides r_{ij} and r_{ik} . The function h is given by:

$$h(r_{ij}^*, r_{ik}^*, \theta_{jik}) = \lambda \cdot \exp\left\{\frac{\gamma}{(r_{ij}^* - a)} + \frac{\gamma}{(r_{ik}^* - a)}\right\} \times (\cos\theta_{jik} + \frac{1}{3})^2, \quad \text{for } r_{ij}^* < a$$

and

$$h(r_{ij}^*, r_{ik}^*, \theta_{jik}) = 0, \quad \text{for } r_{ij}^* \geq a.$$

For a specific system like Si this potential has a total of 9 parameters to be evaluated. ϵ and σ are the energy and distance scaling parameters and the rest of the parameters are dimensionless. The parameter a serves as a cut off function and determines the range of two- as well as three-body interactions. Because the functions cut off smoothly at $r_{ij} = a$ no difficulties are involved in taking proper derivatives for simulation studies. These parameters have been evaluated first by Stillinger and Weber [13] for silicon ensuring that the diamond structure is the most stable periodic arrangement of Si atoms at low temperature. Other criteria used in deciding the best values for parameters were the melting point of Si and the liquid Si structure. Numerical values of seven dimensionless parameters obtained by Stillinger and Weber [13] are: $A = 7.049556277$, $B = 0.6022245584$, $p = 4.0$, $q = 0.0$, $a = 1.80$, $\lambda = 21.0$ and $\gamma = 1.20$. The most commonly used scaling parameters are: $\epsilon = 2.16817\text{eV}$ and $\sigma = 2.0951\text{\AA}$.

4. Among those potential functions we included in this review, the (PTHT) potential has the simplest analytic form [14]. Two-body interactions in this potential are represented by a Lennard-Jones type function:

$$\phi_2 = \sum_i^N \sum_{j < i}^N \epsilon \left[\left(\frac{r_o}{r_{ij}} \right)^{12} - 2 \left(\frac{r_o}{r_{ij}} \right)^6 \right] \quad (4)$$

where, r_{ij} denotes the internuclear distance between the particles i and j ; r_o represents the equilibrium distance and ϵ is the two-body energy at $r_{ij} = r_o$. The three-body part in the (PTHT) potential has been approximated by an Axilrod-Teller type triple dipole function [15]:

$$\phi_3 = \sum_i^N \sum_{j < i}^N \sum_{k < j}^N \frac{Z(1 + 3\cos\theta_i \cos\theta_j \cos\theta_k)}{(r_{ij} \cdot r_{ik} \cdot r_{jk})^3} \quad (5)$$

where, $\theta_i, \theta_j, \theta_k$ and r_{ij}, r_{ik}, r_{jk} represent the angles and the sides of the triangle formed by the three particles i, j and k , respectively. The three-body intensity parameter is denoted by Z . This potential contains only 3 parameters (ϵ, r_o and Z) to be evaluated. For Si these parameters were calculated as $\epsilon = 2.817\text{eV}$, $r_o = 2.2915\text{\AA}$ and $Z = 3484 \text{ eV/\AA}^9$ from fits to the equilibrium distance of Si_2 and the nearest neighbor distance of the equilibrium diamond cubic structure of Si [14]. Furthermore, it was ensured that the diamond cubic is the lowest energy configuration among the common crystalline structures and, at the same time, the stability condition given by $(\partial\Phi/\partial V)_{T=0K} = 0$ is satisfied. As it is expressed here the (PTHT) potential does not intrinsically use a special cut-off function. In computations, however, summations are typically carried out beyond the $3r_o$ limit thereby including up to the sixth coordination shell around a central Si atom.

Comparisons and Discussions

Next, we analyzed comparatively the flexibilities of these functions and assessed their abilities in reproducing properties of Si for bulk, surfaces and small clusters.

Bulk properties calculated by (T), (TD), (SW) and (PTHT) potentials for various structures are tabulated in Table 2. Because the equilibrium volume of diamond cubic Si was used in parameter evaluation procedures, all four potentials reproduce crystalline dimensions of bulk Si(diamond) correctly. The cohesive energy of diamond Si was employed in the parameterization of (T) and (TD) potentials; therefore, these potentials can exactly reproduce the cohesive energy of diamond Si. However, cohesive energy of Si(diamond) calculated by (SW) and (PTHT) potentials (with parameters given in this article) deviate about 7 and 19%, respectively, from the experimental value. Also given in Table 2 are cohesive energy values for the β -tin structure (which is a high pressure form of Si) estimated by (T), (TD), (SW) and (PTHT) potentials. While (TD) potential provides the best value, the result obtain by (T), (SW) and (PTHT) potentials deviate about 3%, 7% and 10%, respectively, from the *ab initio* results [10,11]. Structural properties (such as the atomic volume and c/a ratio) are rather reasonably well predicted by both the (T) as well as the (PTHT) potentials. Unfortunately, values calculated by the (TD) potential for those structural properties were not given in the reference [12]. However, it is anticipated that these values should be quite close to ones obtained by the (T) potential. The cohesive energy and the atomic volume for the β -tin structure calculated by the (SW) potential were taken from Figure 1 of reference [16], while no value for the equilibrium c/a has been found. It appears that the (SW) potential is quite successful in calculating the cohesive energy of the β -tin structure, even though the equilibrium volume was found to be somewhat larger than experimental value. The (SW) potential does not, however, result in the diamond to β -tin phase transformation at high pressures [17]. The cohesive energies calculated by (T) and (TD) potentials for the hypothetical graphitic structure are in

fair agreement with the *ab initio* result obtained by Yin and Cohen [18]. Values obtained by the (SW) and (PTHT) potentials, on the other hand, deviate from this *ab initio* value considerably (see Table 2). While the nearest neighbor distances obtained by the (T) and (PTHT) potentials are in good agreement with the *ab initio* results, the (SW) potential produces a somewhat larger value for the nearest neighbor distance. In analyzing the cohesive energy and other structure related properties of the graphitic form calculated by the (T), (TD) and (SW) potentials, the short range nature of these functions should be kept in mind. Energy calculations performed using these potentials for the graphitic structure, for instance, do not include interactions between atoms located in neighboring planes. This point may become an important issue if one relaxes the graphitic structure in the direction perpendicular to its basal planes. Elastic properties of Si(diamond) at different temperatures have been investigated by Kluge et al., [19] using the (SW) potential. The maximum deviation from the experimental value found in the calculated elastic constants was about 40% for the C_{44} value. This is a very good prediction considering that elastic properties have not been employed in the parameter evaluation of the (SW) function. No comparable study has been conducted for the (T) and (TD) potentials yet. However, both of these potentials in their parameterizations employ the experimental bulk modulus; therefore, elastic constants are expected to be reproduced within acceptable limits by these functions. On the other hand, the bulk modulus calculated by the (PTHT) potential is about 2.5 times larger than the experimental value indicating that the total potential energy curve described by the (PTHT) as a function of the volume is too steep around its minimum region [20]. Melting behavior of Si using the (SW) potential has been investigated by various researchers [13,21-24]. In their original paper Stillinger and Weber [13] using a fixed volume simulation procedure calculated the melting point of Si as 0.08 in reduced units (corresponding to $T_m = 2012$ K). This was also reconfirmed later by Gawlinski and Gunton [21]. Other calculations [22,23], in general, based on fixed pressure procedures produced $T_m \approx 1760$ K. Takai et al. [25,26], using a fixed pressure Monte-Carlo method based on the (PTHT) potential, calculated the melting point as $T_m \approx 2000$ K. Both, (SW) and (PTHT) potentials produced an approximately 5% volume contraction upon melting which is about half of the experimental value [23,25]. At the present time there has been no investigation on the melting behavior of Si employing (T) or (TD) potentials.

Structure and energy values for Si(111) and Si(100) surfaces calculated by (T), (TD) and (PTHT) potentials are given in Table 3, along with some corresponding literature values. For the Si(111) surface, relaxation energies (with respect to the unrelaxed ideal surface) obtained by the (T) and (TD) functions are only slightly lower than the literature values. The (PTHT) potential, in this case, produced an energy value consistent with *ab initio* results. The contraction in the top interlayer spacing of the relaxed Si(111) surface, was correctly predicted by all three potentials. The magnitude of the shrinkage is also equally well predicted by (T), (TD) and (PTHT) potentials. On the relaxed Si(100) surface, (T) and (PTHT) potentials

predict dimerization of Si atoms which is consistent with experimental observations. Also, dimer energies and dimer bond lengths calculated by these potentials agree reasonably well with the literature values. For the (TD) potential Dodson [12] in his paper gives no numerical values for the Si dimer on the Si(100) surface. However, based on Dodson comments, we expect that the dimer energy and the bond length predicted by the (TD) potential should be similar to the (T) potential results. Although the (SW) potential has been used in several computer simulation studies of silicon surfaces, no easily usable numerical values for the relaxation energy and associated structural reconstruction of the Si(111) and Si(100) surfaces have been found. Only, Gawlinski and Gunton [21] in their molecular dynamics study on the epitaxial growth of the Si(100) surface using the (SW) potential, found clear evidence of the dimer formation (see also [22]).

Optimized energies and geometries of small clusters calculated by (T), (TD), (SW) and (PTHT) potentials using parameters given in this report, are tabulated in Table 4. For the dimer case, the energy and the equilibrium distance were correctly reproduced by the (T) potential, because these quantities were employed in the evaluation of parameters. Literature values for the dimer energy and the equilibrium separation were reported as 3.21 eV and 2.246 Å, respectively [27]. For (TD), (SW) and (PTHT) potentials deviations in energy values of Si₂ are 12.5%, -32.4% and -12.1%, while deviations in the equilibrium separation were found to be -2.5%, 4.6% and 2.4%, respectively. For Si₂, accordingly, the equilibrium bond energy and the bond distance are best represented by the (T) potential, while the results obtained by the (SW) potential deviate considerably from the literature values. For the Si₃ case, the energetically most stable structures for the (T) and (SW) potentials were found to be an equilateral triangular shape while (TD) and (PTHT) favored linear configurations. The energy difference between these linear and equilateral triangular states for the (PTHT) potential was found to be 0.08 eV while for the others, i.e., for (T), (TD), and (SW), the energy differences are about 1. eV or more (see Table 1). High level *ab initio* calculations for the Si₃ case predicts an isosceles triangle with an apex bond angle of 80.6° as the ground state [28]. None of the potentials considered in this work can provide this. However, according to a recent article by Koutecky and Fantucci [29], the energy difference between the linear and triangular forms of Si₃ would be too small to be predicted correctly. This is in agreement with the result obtain by the (PTHT) potential. Consistently, for all four cases, calculations produced interatomic distances for the triangular case somewhat larger than the nearest neighbor distances in the linear structures. While the distances calculated by (T), (TD) and (PTHT) were found to be relatively close to each other, (SW) results turned out to be somewhat larger. Optimized results for the Si₄ case are rather interesting. Each of these potential functions produced a different minimum energy structure. The (T) potential produced a three-dimensional regular tetrahedral structure as the lowest state, while the (TD) potential favored a linear chain structure. Planar rhombus and square structures were obtained as the energetically most stable configurations from the (PTHT) and

(SW) potentials, respectively (see Table 4). As in the case of Si_3 , the smallest variations in the optimized energies among different Si_4 geometries was produced by the (PTHT) potential. There are several recent investigations [29,30] on Si_4 supporting the rhombus structure to be the most favorable one, as predicted by the (PTHT) potential.

The (T) potential does a remarkably good job in calculating various energy and structure related properties of bulk Si in different allotropic forms. It has been also used to estimate several point defect energies of Si(diamond). With the exception of the hexagonal site interstitial energy (which was found to be almost zero), calculated results for defect formation have been reported to be in fair agreement with *ab initio* values [9]. In addition to surface results given in Table 3, adatom binding energies on the Si(111) surface have also been calculated by the (T) potential [9]. Results seems to be consistent with *ab initio* calculations. Additionally, for the Si(111) surface, the (T) potential provides the π -bonded chain structure of Pandey [31,32] and at the same time it produces the (7×7) reconstructed Si(111) surface as the energetically most favorable for the Takayanagi model [9]. Even though these results produced by the (T) potential may be open to various criticisms, because the (T) potential produces a metastable Si(diamond) structure (based on Dodson's evaluation [12]), the agreement obtained is quite remarkable.

According to Dodson [12], the (TD) potential predicts correctly the diamond structure for Si to be the most stable structure. Undoubtedly, this is an important improvement, because the (TD) potential also produces several bulk and surface properties of Si with the same accuracy as the (T) potential. In our view, however, the (TD) potential needs further testing. In particular, values for point defects, adatom binding energies and binding sites have not yet been calculated. Furthermore, as indicated above, small cluster results of these two potentials are quite different. In addition to the Si_2 case for which (T) and (TD) potentials produce somewhat different equilibrium bond energies and distances (see table 4), the (TD) potential values for Si_3 and Si_4 cases are considerably different (both energetically and structurally) from the (T) potential results. Neither potential produces an Si_4 configuration consistent with the *ab initio* result. Furthermore, the energy difference between the linear and equilateral triangular configurations of Si_3 calculated by both potentials are quite large [29]. Neither (T) nor (TD) potentials has yet been used to calculate temperature dependent quantities of Si. It will be very interesting to employ these potentials, for instance, for simulating the melting process.

Cohesive energy values calculated by the (SW) potential for different forms of Si are generally somewhat higher than literature values (see Table 2). However, in addition to its ability to predict excellent melting properties, the (SW) potential has been shown to produce acceptable values for the pair correlation function of Si at elevated temperatures [13]. Also, this potential has been used successfully by Kluge et al., [23] to simulate the formation of amorphous silicon by rapid quench-

ing. According to Dodson [17] the (SW) potential produces a vacancy formation energy which agrees well with the *ab initio* result. Also, in the same paper, Dodson employing a Monte-Carlo procedure determined that an epitaxial growth beyond one-third of a monolayer coverage on the Si(111) surface is not well represented by the (SW) function. Contrary to this result, however, molecular dynamics calculations conducted by Schneider et al. [33] produced a well stacked growth and properly crystallized Si structures at some intermediate temperatures. In another molecular dynamics study based on (SW) potential, Gawlinski and Gunton [21] simulated the molecular beam epitaxial growth of the Si(100) surface at different temperatures. Also using the (SW) function Abraham and Broughton [22] analyzed the melting behavior of Si(111) and Si(100) surfaces by a molecular dynamics method. Furthermore, Landmann et al. [24] successfully simulated the melt-Si(100) interface using a molecular dynamics technique based on the (SW) potential. The (SW) potential has also been employed by several investigators to study small clusters of Si. Blaisten-Barojas and Levesque [34] investigated various charged and neutral clusters of Si at the low temperature limit and correlated their findings with the observed "magic numbers". Recently, Feuston et al., [35] using a molecular dynamics technique based on the (SW) function determined finite temperature structures of Si clusters and investigated the fragmentation process. The (SW) potential produces a planar square Si_4 structure as the energetically most stable configuration and favors the equilateral triangular shape trimer more than 1 eV over the linear Si_3 . As indicated in Table 2, the (SW) function produced the largest deviations in the equilibrium energy and bond distance for the dimer among the functions included in this study.

Bulk structural properties are in general well predicted by the (PTHT) potential. Cohesive energies of different Si forms are somewhat overestimated. However, the (PTHT) function correctly predicts the energetically most favorable structure to be the diamond cubic. Despite the fact that it produces a large bulk modulus value, as indicated above, the (PTHT) function has been shown to provide proper absolute stability criteria for the diamond cubic structure [36]. Defect energies calculated by the (PTHT) potential seem to be only in a semi-quantitative agreement with the values reported in the literature. The vacancy and the interstitial energies were calculated as 1.5 and 0.2 eV, respectively, which are considerably lower than the literature values [37]. The (PTHT) potential has been used by the same group in a number of surface related investigations. Computer simulation studies have been conducted successfully to investigate: the effect of surface stress on the reconstruction of the Si(111) surface [38], Si(111) cleavage and the (2×1) reconstruction process [39], long range ledge-ledge interaction on Si(111) surfaces [40], adatom diffusion and adatom-ledge interactions on the Si(111) surface [41], and kink site formation energies on the Si(111) surface [42]. In these studies the level of success extends from quantitative to qualitative levels when compared with the limited number of available experimental results. In general, it is fair to say that structural properties of surfaces are reasonably well predicted by the (PTHT) func-

tion. Although the equilibrium bond energy obtained by the (PTHT) potential deviates about 12% from its literature value for the gas-phase Si dimer, it produces the bond distance of Si₂ within acceptable limits. This potential, like the (TD) function, favors the linear Si₃ configuration. However, the (PTHT) produces a very small energy difference between the triangular and the linear forms of Si₃ which is consistent with the prediction by Koutecky and Fantucci based on *ab initio* considerations [29]. A rhombus structure for Si₄ was predicted by the (PTHT) function to be the energetically most stable configuration that is also consistent with reported *ab initio* results [28,29].

As anticipated, the type of potential energy functions used in a modeling procedure dictates many calculated properties of a system. One of the features most desired of a model potential function is its transferability. This means that the same potential function with the same parameters is able to describe various properties of a system in different forms [9]. The evaluation of parameters of a model potential function is a time consuming and cumbersome job. The difficulty, in general, increases with the increasing number of parameters to be determined. On the other hand, a function with many adjustable parameters is expected to do a better job in reproducing different properties along with a better transferability. Perhaps, because of the limited number of samplings considered in the present comparison, potentials containing more parameters do not necessarily produce remarkably better results.

Conclusions

Structural properties of bulk Si are equally well predicted by all four potential functions considered in this report. Cohesive energies of different bulk forms are best represented by (T) and (TD) functions, while calculations based on (SW) and (PTHT) functions exhibit some deviations. Bulk moduli of silicon estimated using (T), (TD) and (SW) potentials agree well with values reported in the literature. However, the (PTHT) function produces a bulk modulus which agrees only qualitatively with the experiment. The melting point and the change in volume upon melting of Si, are well predicted by both (SW) and (PTHT) functions. High temperature properties of Si, including the melting behavior, however, are not yet available for (T) and (TD) potentials. Reconstruction patterns and energetics of Si(111) and Si(100) surfaces were reasonably well predicted by (T), (TD) and (PTHT) potentials while no calculations for the same properties were found for the (SW) function. This conclusion on the predictive power of these functions, however, must be treated with caution, because the present comparison is based only on a limited number of calculations which are available in the literature for more than one type of potential function. Small cluster properties (for Si₃ and Si₄, in particular) appear to be best reproduced by the (PTHT) function while the (T) potential provides the best result for the Si₂ case.

References

- [1] F. F. Abraham, J. Vac. Scie. Technol., **B 2**, 534 (1984).
- [2] J. N. Murrell, S. Carter, S. C. Farantos, P. Huxley and A. J. C. Varandas, *Molecular Potential Energy Functions*, (John Wiley, New York, 1984).
- [3] C. Hoheisel, Phys. Rev., **A 23**, 1998 (1981).
- [4] L. Verlet, Phys. Rev., **159**, 98 (1967).
- [5] A. Rahman, Phys. Rev., **136**, A405 (1964).
- [6] T. Halicioglu, H. O. Pamuk and S. Erkoc, Surf. Scie., **143**, 601 (1984).
- [7] T. Halicioglu, T. Takai and W. A. Tiller, "The Structure of Surfaces", Eds: M. A. Van Hove and S. Y. Tong (Springer Verlag, 1985) pp. 231.
- [8] L. G. M. Pettersson, C. W. Bauschlicher, Jr., and T. Halicioglu, J. Chem. Phys., **87**, 2205 (1987).
- [9] J. Tersoff, Phys. Rev. Lett., **56**, 632 (1986).
- [10] M. T. Yin and M.L. Cohen, Phys. Rev. Lett., **45**, 1004 (1980).
- [11] M. T. Yin and M.L. Cohen, Phys. Rev., **B 26**, 5668 (1982).
- [12] B. W. Dodson, Phys. Rev., **B 35**, 2795 (1987).
- [13] F. H. Stillinger and T. A. Weber, Phys. Rev., **B 31**, 5262 (1985).
- [14] E. Pearson, T. Takai, T. Halicioglu and W. A. Tiller, J. Cryst. Growth, **70**, 33 (1984).
- [15] T. Halicioglu, Phys. Stat. Sol., (b) **99**, 347 (1980).
- [16] R. Biswas and D. R. Hamann, Phys. Rev. Lett., **55**, 2001 (1985).
- [17] B. W. Dodson, Phys. Rev., **B 33**, 7361 (1986).
- [18] M. T. Yin and M.L. Cohen, Phys. Rev., **B 29**, 6996 (1984).
- [19] M. D. Kluge, J. R. Ray and A. Rahman, J. Chem Phys., **85**, 4028 (1986).
- [20] E. M. Pearson, Ph.D. Thesis, (Stanford University, Department of Materials

Science and Engineering, 1985).

- [21] E. T. Gawlinski and J. D. Gunton, Phys. Rev., **B 36**, 4774 (1987).
- [22] F. F. Abraham and J. Q. Broughton, Phys. Rev Lett., **56**, 734 (1986).
- [23] M. D. Kluge, J. R. Ray and A. Rahman, Phys. Rev., **B 36**, 4234 (1987).
- [24] U. Landman, W. D. Luedtke, R. N. Barnett, C. L. Cleveland, M. W. Ribarsky, E. Arnold, S. Ramesh, H. Baumgart, A. Martinez and B. Khan, Phys. Rev. Lett., **56**, 155 (1986).
- [25] T. Takai, T. Halicioglu and W. A. Tiller, Script. Metall., **19**, 709 (1985).
- [26] T. Takai, Ph.D. Thesis, (Stanford University, Department of Materials Science and Engineering, 1984).
- [27] K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure*, IV, (Van Nostrand Reinhold Co., New York, 1979) .
- [28] K. Raghavachari, J. Chem. Phys., **84**, 5672 (1986).
- [29] J. Koutecky and P. Fantucci, Chem. Rev., **86**, 539 (1986).
- [30] W. L. Brown, R. R. Freeman, K. Raghavachari and M. Schluter, Science, **235**, 860 (1987).
- [31] K. C. Pandey, Phys. Rev. Lett., **47**, 1913 (1981).
- [32] K. C. Pandey, Phys. Rev. Lett., **49**, 223 (1982).
- [33] M. Schneider, I. K. Schuller and A. Rahman, Phys. Rev., **B 36**, 1340 (1987).
- [34] E. Blaisten-Barojas and D. Levesque, Phys. Rev., **B 34**, 3910 (1986).
- [35] B. P. Feuston, R. K. Kalia and P. Vashista, Phys. Rev., **B 35**, 6222 (1987).
- [36] T. Takai, T. Halicioglu and W. A. Tiller, Script. Metall., **19**, 715 (1985).
- [37] S. Oh, Ph.D. Thesis, (Stanford University, Department of Materials Science and Engineering, 1987), Chapter 3.
- [38] E. M. Pearson, T. Halicioglu and W. A. Tiller, Surf. Scie., **168**, 46 (1986).
- [39] E. M. Pearson, T. Halicioglu and W. A. Tiller, J. Vac. Scie. Technol., **A 5**, 293 (1987).

- [40] E. M. Pearson, T. Halicioglu and W. A. Tiller, Surf. Scie., **184**, 401 (1987).
- [41] E. M. Pearson, T. Halicioglu and W. A. Tiller, J. Crystal Growth, **83**, 499 (1987).
- [42] E. M. Pearson, T. Halicioglu and W. A. Tiller, J. Crystal Growth, **83**, 502 (1987).
- [43] "JANAF Thermodynamical Tables", Second Edition (U.S. Department of Commerce, NBS, 1971).
- [44] R. W. G. Wyckoff, "Crystal Structures", Vol 1, Second Edition (John-Wiley, New York, 1963).
- [45] J. Donohue, "The Structures of Elements", (John-Wiley, New York, 1974).
- [46] J. E. Northrup and M. L. Cohen, Phys. Rev. Lett., **47**, 1910 (1981).
- [47] J. E. Northrup and M. L. Cohen, Phys. Rev. Lett., **49**, 1349 (1982).
- [48] W. S. Verwoerd and F. J. Kok, Surf. Scie., **80**, 89 (1979).
- [49] M. T. Yin and M.L. Cohen, Phys. Rev., **B 24**, 2303 (1981).
- [50] C. Pandey, in "Proc. of the 7th International Conf. on the Physics of Semiconductors". Eds: D. J. Chadi and W. A. Harrison (Springer Verlag, New York, 1985), pp. 55.

Table 1. Parameters of the Tersoff (T) and Tersoff-Dodson (TD) Potentials for Silicon [9,12].

Parameters	Tersoff (T)	Tersoff-Dodson (TD)	Units
A	2280.0	1614.6	(eV)
B_o	171.0	155.08	(eV)
λ_1	2.930	2.7793	(\AA^{-1})
λ_2	1.465	1.3969	(\AA^{-1})
n	4.0	4.0	
b	1.324	3.4785	
η	1.0	0.6207	
c	6.50	0.8543	
d	6.02	3.9588	
R	3.0	3.0	(\AA)
D	0.2	0.2	(\AA)

Table 2. Bulk properties of silicon calculated by (T), (TD), (SW) and (PTHT) potentials.

	(T)	(TD)	(SW)	(PTHT)	Literature Values
Diamond Structure Cohesive Energy (eV)	-4.63	-4.63	-4.34	-5.57	-4.66 [43]
Diamond Structure Atomic Volume (\AA^3)	20.02	20.02	20.02	20.02	20.02 [43,44]
β -tin Structure Cohesive Energy (eV)	-4.51	-4.28	-4.05	-4.82	-4.36 [10,11]
β -tin Structure c/a Ratio	0.52	(*)	(*)	0.546	0.55 [10,11,45]
β -tin Structure Atomic Volume (\AA^3)	15.7	(*)	17.5	16.28	15.5 [10,11] 14.19 [45]
Graphite Structure Cohesive Energy (eV)	-4.30	-4.24	-3.14	-5.14	-3.92 [18]
Graphite Structure Nearest Neighbor Distance (\AA)	2.28	(*)	2.37	2.214	2.25 [18]

(*) No calculations are available for these cases.

Table 3. Surface properties of Si calculated by (T), (TD) and (PHT) potentials.

	(T)	(TD)	(PHT)	Literature Value
Si(111) Energy of Relaxation (eV/atom)	0.12	0.12	0.166	0.15-0.17 [46,47]
Si(111) Contraction in the first interlayer spacing (%)	29.	30.	27.	25.-37 [31,32,46-48]
Si(100) Internuclear distance in the Si ₂ dimer (Å)	2.29	(*)	2.31	2.22-2.25 [49,50]
Si(100) Dimerization energy (eV/dimer)	1.9	(*)	2.29	1.7-2.1 [49,50]

(*) no calculations were found for these cases.

Table 4. Small cluster properties of Si calculated by (T), (TD), (SW) and (PTHT) functions. Total binding energies and minimum distances were denoted by E_b and r_{min} , respectively.

	(T)		(TD)		(SW)		(PTHT)	
	E_b (eV)	r_{min} (Å)	E_b (eV)	r_{min} (Å)	E_b (eV)	r_{min} (Å)	E_b (eV)	r_{min} (Å)
Si ₂	3.21	2.24	3.61	2.19	2.17	2.35	2.82	2.30
Si ₃ <i>linear</i>	6.40	2.24	7.04	2.20	3.38	2.42	6.25	2.27
Si ₃ <i>triangular</i>	7.64	2.32	6.05	2.40	4.44	2.56	6.17	2.39
Si ₄ <i>linear</i>	9.60	2.24	10.48	2.20	5.49	2.41	9.76	2.25
Si ₄ <i>square</i>	10.48	2.31	9.73	2.34	8.14	2.39	9.97	2.34
Si ₄ <i>rhombus</i>	11.90	2.34	9.53	2.40	(*)		10.02	2.37
Si ₄ <i>tetrahedron</i>	12.13	2.40	8.86	2.51	6.67	2.71	9.17	2.48

(*) No minimum was found for this configuration interacting via (SW) potential.